FEFF

FEFF is an automated program for ab initio multiple scattering calculations of X-ray Absorption Fine Structure (XAFS), X-ray Absorption Near-Edge Structure (XANES) and various other spectra for clusters of atoms. The code yields scattering amplitudes and phases used in many modern XAFS analysis codes, as well as various other properties.

For more information: https://feff.phys.washington.edu/feffproject-feff.html

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